

## Multiplicity Factors of Crystal Planes for 21 Noncentrosymmetric Point Groups (for the Powder Method)

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The multiplicity factor, which is defined as the number of different planes in a form having identical interplanar spacing and identical intensity, is tabulated here for the 21 noncentrosymmetric point groups on the basis of their symmetries.

### Introduction

The multiplicity factor is one of the six factors affecting the relative intensity of the diffraction lines on a powder pattern (Cullity, 1978).

For all crystals not containing an anomalous scatterer and for a centrosymmetric crystal containing an anomalous scatterer, their intensities  $I(hkl)$  have the symmetry of a centrosymmetric point group, i. e., Friedel symmetry, and their multiplicity factors have been reported in many literature references (Nuffield, 1966; Azaroff, 1968; Henry & Lonsdale, 1969; Klug & Alexander, 1974; Cullity, 1978).

For a noncentrosymmetric crystal containing an anomalous scatterer, however,

Friedel's law does not hold, and the multiplicity factors of their crystal planes reported so far are incomplete and even contain error (Hahn, 1992).

In this paper, the multiplicity factors for all crystal forms of twenty one noncentrosymmetric point groups are tabulated rather clearly.

### Theory

The 32 point groups are divided among the seven crystal systems. Eleven point groups are centrosymmetric and the remaining 21 are noncentrosymmetric. In the trigonal system there exist three noncentric point groups,  $3(R)$ ,  $32(R)$  and  $3m(R)$ . They are compatible with a rhombohedral lattice as well as with a hexagonal lattice.

Furthermore, the point groups 32 and 3m in the hexagonal description are subdivided into two cases each - one having the 2-fold symmetry axis of the point group 32 and the normal of the mirror plane of the point group 3m in the orientation [100], and the other one having them in the [210] direction. The point group  $\bar{6}m2$  in the hexagonal system can be also described as  $\bar{6}2m$

The point groups 2 and m belonging to the monoclinic system are subdivided into two cases each - with the b-axis unique and with the c-axis unique. Therefore 21 point groups are classified into 28 different kinds in Table 1.

Since the distribution of the crystallographic reciprocal lattice points shows the same symmetry as a real crystal lattice of the corresponding point group, the equivalent plane reflections of each point

group are derived by the operation of its symmetry to the general Miller index hkl.

There are 14 different kinds of planes for positive Miller indices :hkl, hkh, hkk, hhl, hhh, 0kl, h0l, hk0, 0kk, h0h, hh0, h00, 0k0, 00l. The substitutions of these planes into the equivalent plane relation results in the multiplicity factors for the crystal forms.

Table 1 gives the 28 different kinds of point groups (column 2).

The crystal system is given in column 1. Column 3 shows symmetrically equivalent planes whose number corresponds to the multiplicity factors given in the last column.

One should notice that even for non-centrosymmetric crystals the diffraction lines for pairs of reflections  $hkl$  and  $\bar{h}\bar{k}\bar{l}$  coincide in a powder patterns.

**Table 1.** Multiplicity factors of crystal planes for 21 noncentrosymmetric point groups, R: rhombohedral coordinate axis, H: hexagonal coordinate axis

System	Point groups	Miller indices	Multiplicity factor
Tri- clinic	1	all planes	1
Mono- clinic	2 (b-axis unique)	0k0 0 $\bar{k}$ 0	1
		The rest	2
	m (b-axis unique)	$h0l \bar{h}0l h0\bar{l} \bar{h}0\bar{l} h0h \bar{h}0h h0\bar{h} \bar{h}0\bar{h} h00 \bar{h}00 00l 00\bar{l}$	1
		The rest	2
	2 (c-axis unique)	00l 00 $\bar{l}$	1
		The rest	2
m (c-axis unique)	$hk0 \bar{h}k0 h\bar{k}0 \bar{h}\bar{k}0 hh0 \bar{h}h0 h\bar{h}0 \bar{h}\bar{h}0 h00 \bar{h}00 0k0 0\bar{k}0$	1	
	The rest	2	
Ortho- rhom- bic	222	$h00=\bar{h}00 0k0=0\bar{k}0 00l=00\bar{l}$	2
	(22)	The rest	4

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	$mm2$ ( $mm$ )	$00l\ 00\bar{l}$	1	
		$h0l=\bar{h}0l\ 0kl=0\bar{k}l\ 0k\bar{l}=0\bar{k}\bar{l}\ 0kk=0\bar{k}k\ 0k\bar{k}=0\bar{k}\bar{k}$ $h0\bar{l}=\bar{h}0\bar{l}\ h0h=\bar{h}0h\ h0\bar{h}=\bar{h}0\bar{h}\ h00=\bar{h}00\ 0k0=0\bar{k}0$	2	
		The rest	4	
Tetra- gonal	4	$00l\ 00\bar{l}$	1	
		The rest	4	
	$\bar{4}$	$00l=00\bar{l}$	2	
		The rest	4	
	422 (42)	$00l=00\bar{l}$	2	
		$hh0=\bar{h}h0=h\bar{h}0=\bar{h}\bar{h}0\ h00=\bar{h}00=0h0=0\bar{h}0$	4	
		The rest	8	
	4mm (4m)	$00l\ 00\bar{l}$	1	
		$hhl=h\bar{h}l=\bar{h}hl=\bar{h}\bar{h}l\ \ hhh=h\bar{h}h=\bar{h}hh=\bar{h}\bar{h}h$ $h\bar{h}l=h\bar{h}\bar{l}=\bar{h}hl=\bar{h}\bar{h}\bar{l}\ \ hh\bar{h}=h\bar{h}h=\bar{h}h\bar{h}=\bar{h}\bar{h}h$ $h0l=\bar{h}0l=0hl=0\bar{h}l\ \ h0h=\bar{h}0h=0hh=0\bar{h}h$ $h0\bar{l}=\bar{h}0\bar{l}=0h\bar{l}=0\bar{h}\bar{l}\ \ h0\bar{h}=\bar{h}0\bar{h}=0h\bar{h}=0\bar{h}\bar{h}$ $h00=\bar{h}00=0h0=0\bar{h}0\ \ hh0=h\bar{h}0=\bar{h}h0=\bar{h}\bar{h}0$	4	
		The rest	8	
		$\bar{4}2m$ (42)	$00l=00\bar{l}$	2
			$hhl=\bar{h}hl=h\bar{h}l=\bar{h}\bar{h}l\ \ hhh=\bar{h}h\bar{h}=h\bar{h}h=\bar{h}\bar{h}h$ $h\bar{h}l=\bar{h}hl=h\bar{h}\bar{l}=\bar{h}\bar{h}\bar{l}\ \ hh\bar{h}=\bar{h}hh=h\bar{h}h=\bar{h}\bar{h}h$ $h00=\bar{h}00=0h0=0\bar{h}0\ \ hh0=\bar{h}h0=h\bar{h}0=\bar{h}\bar{h}0$	4
The rest	8			
$\bar{4}m2$ (4m)	$00l=00\bar{l}$	2		
	$0kl=0\bar{k}l=k0\bar{l}=\bar{k}0\bar{l}\ \ 0kk=0\bar{k}k=k0\bar{k}=\bar{k}0\bar{k}$ $h0l=\bar{h}0l=0hl=0\bar{h}l\ \ h0h=\bar{h}0h=0hh=0\bar{h}h$ $h00=\bar{h}00=0h0=0\bar{h}0\ \ hh0=h\bar{h}0=\bar{h}h0=\bar{h}\bar{h}0$	4		
	The rest	8		
Tri- gonal	3(R)	$hhh\ \bar{h}\bar{h}h$	1	
		The rest	3	
	3(H)	$00l\ 00\bar{l}$	1	
		The rest	3	
	32(R)	$hhh=\bar{h}\bar{h}h$	2	
		$\bar{h}h0=0\bar{h}h=h0\bar{h}\ \ h\bar{h}0=0h\bar{h}=\bar{h}0h$	3	
		The rest	6	
	321(H)	$00l=00\bar{l}$	2	
		$hh0=h2\bar{h}0=2\bar{h}h0\ \ \bar{h}\bar{h}0=\bar{h}2h0=2h\bar{h}0$	3	
		The rest	6	

	312(H)	$00l=00\bar{l}$	2
		$h00=0\bar{h}0=\bar{h}h0 \quad \bar{h}00=0h0=h\bar{h}0$	3
		The rest	6
	3m(R)	$hhh \quad \bar{h}\bar{h}\bar{h}$	1
		$hkh=khh=hkh \quad \bar{h}k\bar{h}=\bar{k}\bar{h}\bar{h}=\bar{h}hk \quad h\bar{k}h=\bar{k}hh=h\bar{h}\bar{k}$ $\bar{h}\bar{k}\bar{h}=\bar{k}h\bar{h}=\bar{h}hk \quad h0h=0hh=h00 \quad \bar{h}0\bar{h}=0\bar{h}\bar{h}=\bar{h}\bar{h}0$ $\bar{h}hh=h\bar{h}\bar{h}=h\bar{h}\bar{h} \quad \bar{h}\bar{h}h=\bar{h}\bar{h}\bar{h}=h\bar{h}\bar{h} \quad h00=0h0=00h$ $\bar{h}00=0\bar{h}0=00\bar{h}$	3
		The rest	6
	3m1(H)	$00l \quad 00\bar{l}$	1
		$\bar{h}hh=h0h=0\bar{h}h \quad \bar{h}\bar{h}\bar{h}=h0\bar{h}=0\bar{h}\bar{h} \quad h\bar{h}h=\bar{h}0h=0hh$ $h\bar{h}\bar{h}=\bar{h}0\bar{h}=0\bar{h}\bar{h} \quad h0l=0\bar{h}l=\bar{h}hl \quad \bar{h}0l=0hl=h\bar{h}l$ $\bar{h}0\bar{l}=0h\bar{l}=\bar{h}h\bar{l} \quad h0\bar{l}=0\bar{h}\bar{l}=\bar{h}h\bar{l} \quad h00=0h0=\bar{h}h0$ $\bar{h}00=0\bar{h}0=h\bar{h}0$	3
		The rest	6
	31m(H)	$00l \quad 00\bar{l}$	1
		$hhl=h2\bar{h}l=2\bar{h}hl \quad \bar{h}hl=\bar{h}2hl=2h\bar{h}l$ $h\bar{h}l=h2\bar{h}l=2\bar{h}h\bar{l} \quad \bar{h}\bar{h}l=\bar{h}2h\bar{l}=2h\bar{h}\bar{l}$ $hhh=h2\bar{h}h=2\bar{h}hh \quad \bar{h}hh=\bar{h}2hh=2h\bar{h}h$ $h\bar{h}\bar{h}=h2\bar{h}\bar{h}=2\bar{h}h\bar{h} \quad \bar{h}\bar{h}\bar{h}=\bar{h}2h\bar{h}=2h\bar{h}\bar{h}$ $hh0=h2\bar{h}0=2\bar{h}h0 \quad \bar{h}h0=\bar{h}2h0=2h\bar{h}0$	3
		The rest	6
Hexagonal	6	$00l \quad 00\bar{l}$	1
		The rest	6
	$\bar{6}$ (3/m)	$00l=00\bar{l}$	2
		$hk0=\bar{h}+\bar{k}h0=k\bar{h}+\bar{k}0 \quad h\bar{k}0=\bar{h}+kh0=\bar{k}\bar{h}+k0$ $\bar{h}k0=h+k\bar{h}0=kh+\bar{k}0 \quad \bar{h}\bar{k}0=\bar{h}+kh0=\bar{k}\bar{h}+k0$ $h00=0\bar{h}0=\bar{h}h0 \quad \bar{h}00=0h0=h\bar{h}0$	3
		The rest	6
	622 (62)	$00l=00\bar{l}$	2
		$hh0=2h\bar{h}0=h2\bar{h}0=\bar{h}\bar{h}0=2\bar{h}h0=\bar{h}2h0$ $h00=\bar{h}00=0h0=0\bar{h}0=\bar{h}h0=h\bar{h}0$	6
		The rest	12
6mm (6m)	$00l \quad 00\bar{l}$	1	
	$hhl=2h\bar{h}l=h2\bar{h}l=\bar{h}\bar{h}l=2\bar{h}hl=\bar{h}2hl$ $\bar{h}hl=0hl=h0l=h\bar{h}l=0\bar{h}l=\bar{h}0l$ $h\bar{h}l=2h\bar{h}l=h2\bar{h}l=\bar{h}\bar{h}l=2\bar{h}hl=\bar{h}2hl$ $\bar{h}h\bar{l}=0h\bar{l}=h0\bar{l}=\bar{h}\bar{h}\bar{l}=0\bar{h}\bar{l}=\bar{h}0\bar{l}$ $hhh=2h\bar{h}h=h2\bar{h}h=\bar{h}\bar{h}h=2\bar{h}hh=\bar{h}2hh$ $\bar{h}hh=0hh=h0h=h\bar{h}h=0\bar{h}h=\bar{h}0h$ $h\bar{h}\bar{h}=2h\bar{h}\bar{h}=h2\bar{h}\bar{h}=\bar{h}\bar{h}\bar{h}=2\bar{h}h\bar{h}=\bar{h}2h\bar{h}$ $\bar{h}h\bar{h}=0h\bar{h}=h0\bar{h}=h\bar{h}\bar{h}=0\bar{h}\bar{h}=\bar{h}0\bar{h}$	6	

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		$hh0=2h\bar{h}0=h2\bar{h}0=\bar{h}h0=2\bar{h}h0=\bar{h}2h0$ $h00=0h0=\bar{h}00=0\bar{h}0=\bar{h}h0=hh0$		
		The rest	12	
	$\bar{6}m2$ (6m)	$00l=00\bar{l}$		2
		$h00=\bar{h}h0=0\bar{h}0$ $h00=h\bar{h}0=0h0$		3
		$hk0=\bar{h}+k\bar{h}0=k\bar{h}+\bar{k}0=\bar{h}h+k0=h+k\bar{k}0=\bar{k}h0$ $\bar{h}k0=h+k\bar{h}0=k\bar{h}+\bar{k}0=\bar{h}h+k0=\bar{h}+k\bar{k}0=k\bar{h}0$ $h\bar{k}0=\bar{h}+k\bar{h}0=\bar{k}h+k0=\bar{h}h+\bar{k}0=h+k\bar{k}0=k\bar{h}0$ $\bar{h}k0=h+k\bar{h}0=\bar{k}h+k0=\bar{h}h+\bar{k}0=\bar{h}+k\bar{k}0=k\bar{h}0$ $h0l=\bar{h}hl=0\bar{h}l=\bar{h}h\bar{l}=0\bar{h}l=h0\bar{l}$ $\bar{h}0l=h\bar{h}l=0\bar{h}l=h\bar{h}\bar{l}=0\bar{h}l=\bar{h}0\bar{l}$ $h0h=\bar{h}hh=0\bar{h}h=\bar{h}h\bar{h}=0\bar{h}h=h0\bar{h}$ $\bar{h}0h=h\bar{h}h=0\bar{h}h=h\bar{h}\bar{h}=0\bar{h}h=\bar{h}0\bar{h}$ $hh0=2\bar{h}h0=h2\bar{h}0=\bar{h}2h0=2h\bar{h}0=\bar{h}h0$		6
		The rest	12	
	$\bar{6}2m$ (62)	$00l=00\bar{l}$		2
		$hh0=2\bar{h}h0=h2\bar{h}0$ $\bar{h}h0=2h\bar{h}0=\bar{h}2h0$		3
		$hk0=\bar{h}+k\bar{h}0=k\bar{h}+\bar{k}0=h\bar{h}+\bar{k}0=\bar{h}+k\bar{k}0=k\bar{h}0$ $\bar{h}k0=h+k\bar{h}0=k\bar{h}+\bar{k}0=\bar{h}h+\bar{k}0=h+k\bar{k}0=k\bar{h}0$ $h\bar{k}0=\bar{h}+k\bar{h}0=\bar{k}h+k0=\bar{h}h+k0=\bar{h}+k\bar{k}0=\bar{k}h0$ $\bar{h}k0=h+k\bar{h}0=\bar{k}h+k0=\bar{h}h+k0=h+k\bar{k}0=\bar{k}h0$ $hhl=2\bar{h}h\bar{l}=h2\bar{h}\bar{l}=h\bar{h}\bar{l}=2\bar{h}h\bar{l}=h2\bar{h}\bar{l}$ $\bar{h}h\bar{l}=2h\bar{h}\bar{l}=\bar{h}2h\bar{l}=\bar{h}h\bar{l}=2h\bar{h}\bar{l}=\bar{h}2h\bar{l}$ $hhh=2\bar{h}h\bar{h}=h2\bar{h}h=h\bar{h}\bar{h}=2\bar{h}h\bar{h}=h2\bar{h}h$ $\bar{h}h\bar{h}=2h\bar{h}\bar{h}=\bar{h}2hh=h\bar{h}h=2h\bar{h}h=\bar{h}2h\bar{h}$ $h00=\bar{h}00=0h0=0\bar{h}0=\bar{h}h0=h\bar{h}0$		6
		The rest	12	
Cubic	23	$hhh=h\bar{h}h=\bar{h}h\bar{h}=\bar{h}h\bar{h}$ $\bar{h}h\bar{h}=\bar{h}h\bar{h}=h\bar{h}h=h\bar{h}h$	4	
		$h00=0h0=00h=\bar{h}00=0\bar{h}0=00\bar{h}$	6	
		The rest	12	
	432	$h00=0h0=00h=\bar{h}00=0\bar{h}0=00\bar{h}$		6
		$hhh=h\bar{h}h=h\bar{h}h=h\bar{h}h=\bar{h}h\bar{h}=\bar{h}h\bar{h}=h\bar{h}h=h\bar{h}h$		8
		$h0h=\bar{h}0h=h0\bar{h}=\bar{h}0\bar{h}=hh0=\bar{h}h0$ $=h\bar{h}0=\bar{h}h0=0hh=0\bar{h}h=0h\bar{h}=0\bar{h}h$		12
		The rest	24	
	$\bar{4}3m$	$hhh=\bar{h}h\bar{h}=\bar{h}h\bar{h}=\bar{h}h\bar{h}$ $\bar{h}h\bar{h}=\bar{h}h\bar{h}=h\bar{h}h=h\bar{h}h$		4
		$h00=0h0=00h=\bar{h}00=0\bar{h}0=00\bar{h}$		6
		$hkh=\bar{h}k\bar{h}=\bar{h}k\bar{h}=h\bar{k}h=hkh=\bar{h}h\bar{k}$ $=\bar{h}h\bar{k}=h\bar{k}h=k\bar{h}h=\bar{k}h\bar{h}=\bar{k}h\bar{h}=k\bar{h}h$ $\bar{h}k\bar{h}=\bar{h}k\bar{h}=h\bar{k}h=\bar{h}k\bar{h}=hkh=h\bar{h}k$ $=h\bar{h}k=\bar{h}h\bar{k}=\bar{k}h\bar{h}=k\bar{h}h=k\bar{h}h=\bar{k}h\bar{h}$ $hh0=\bar{h}h0=h\bar{h}0=\bar{h}h0=h0h=\bar{h}0h$ $=h0\bar{h}=\bar{h}0\bar{h}=0hh=0\bar{h}h=0h\bar{h}=0\bar{h}h$		12
The rest		24		

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